2-Amino-1-naphthalenesulfonic acid
81-16-3 | DTXSID7020922

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 187 °C

Global applicability domain: Inside

Local applicability domain index: 4.21e-01

Confidence level: 4.58e-01

Nearest Neighbors from the Training Set

Image not found
2-Amino-1-naphthalenesulfonic acid
Measured: 180
Predicted: 187

Image not found
Benzenesulfonic acid, 4-(phenylamino)-
Measured: 206
Predicted: 196

Image not found
6-Hydroxynaphthalene-2-sulfonic acid
Measured: 125
Predicted: 128

Image not found
5-Quinolinesulfonic acid, 8-hydroxy-
Measured: 323
Predicted: 197

Image not found
Sulfabenz
Measured: 200
Predicted: 194